4-Bromo-5-methoxy-3-[(propan-2-yl)oxy]-N-(2H-tetrazol-5-yl)thiophene-2-carboxamide

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 1.04e-11 cm3/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.36e-01

Confidence level: 8.35e-01

Nearest Neighbors from the Training Set

Image not found
Dimethyl adipate
Measured: 8.40e-12
Predicted: 6.84e-12

Image not found
Isoproturon
Measured: 1.20e-11
Predicted: 3.23e-11

Image not found
Dimethyl glutarate
Measured: 3.30e-12
Predicted: 3.76e-12

Image not found
Bornyl acetate
Measured: 1.39e-11
Predicted: 1.36e-11

Image not found
2-Ethoxyethyl methacrylate
Measured: 2.80e-11
Predicted: 2.95e-11